



# **STIC Search Report**

## **Biotech-Chem Library**

**STIC Database Tracking Number: 168193**

**TO: Rei-Tsang Shiao**  
**Location: 5a10 / 5c18**  
**Monday, October 17, 2005**  
**Art Unit: 1626**  
**Phone: 571-272-0707**  
**Serial Number: 10 / 715029**

**From: Jan Delaval**  
**Location: Biotech-Chem Library**  
**Remsen 1a51**  
**Phone: 571-272-2504**  
  
**jan.delaval@uspto.gov**

### **Search Notes**

=> d his

(FILE 'HOME' ENTERED AT 07:16:36 ON 17 OCT 2005)  
SET COST OFF

FILE 'HCAPLUS' ENTERED AT 07:16:46 ON 17 OCT 2005

L1 1 S US20040106807/PN OR (US2003-715029# OR WO2003-US36685 OR US20  
E SONG/AU  
L2 2 S E3  
E SONG J/AU  
L3 370 S E3,E13,E14  
L4 229 S E11  
E SONG JIN/AU  
L5 23 S E3,E29  
E SONG JINHUA/AU  
L6 27 S E3,E4  
E TAN/AU  
L7 1 S E3  
E TAN Z/AU  
L8 69 S E3,E13  
E TAN SHU/AU  
E TAN ZHU/AU  
L9 1 S E3  
L10 11 S E14  
E YEE/AU  
E YEE N/AU  
L11 61 S E3-E5,E8-E11  
SEL RN L1

FILE 'REGISTRY' ENTERED AT 07:19:35 ON 17 OCT 2005

L12 4 S E1-E4

FILE 'HCAPLUS' ENTERED AT 07:20:23 ON 17 OCT 2005

L13 768 S L2-L11 NOT L1  
L14 35 S L13 AND (BOEHRIN? OR BOHRIN?)/PA,CS  
L15 3 S L13 AND BENZEN?/SC,SX  
L16 1 S L13 AND GRIGNARD  
E GRIGNARD/CT  
L17 19700 S E8+OLD,NT OR E13+OLD,NT OR E20+OLD,NT OR E22+OLD,NT  
L18 9760 S E3-E29  
E E8+ALL  
E E8+ALL  
L19 4 S L13 AND L17,L18  
L20 36 S L14-L16,L19  
SEL RN

FILE 'REGISTRY' ENTERED AT 07:25:06 ON 17 OCT 2005

L21 606 S E1-E606  
L22 8 S L21 AND MG/ELS  
L23 8 S L21 AND LI/ELS  
L24 126 S L21 AND C6-C6/ES  
L25 71 S L24 AND C6/ES  
L26 STR  
L27 0 S L26 CSS  
L28 STR L26  
L29 0 S L28 CSS  
L30 STR L28  
L31 1 S L30 CSS

FILE 'CASREACT' ENTERED AT 07:44:50 ON 17 OCT 2005

L32 STR  
L33 0 S L32 CSS  
L34 SCR 1120  
L35 0 S L32 AND L34 CSS SAM  
L36 SCR 1918  
L37 1 S L32 AND L34 AND L36 CSS SAM  
L38 SCR 1989 OR 1990  
L39 0 S L32 AND L34 AND L38 CSS SAM  
L40 SCR 1989 AND 1990  
L41 0 S L32 AND L34 AND L40 CSS SAM  
L42 0 S L32 AND L34 AND L40 SAM  
L43 1 S L32 AND L34 AND L38 SAM  
L44 1 S L1  
L45 13 S ?MGLI?  
L46 0 S L32 SAM SUB=L45

FILE 'REGISTRY' ENTERED AT 07:57:57 ON 17 OCT 2005

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SET SMARTSELECT OFF

FILE 'REGISTRY' ENTERED AT 07:57:59 ON 17 OCT 2005

FILE 'CASREACT' ENTERED AT 07:58:10 ON 17 OCT 2005  
SET SMARTSELECT ON  
SET SMARTSELECT OFF

FILE 'REGISTRY' ENTERED AT 07:58:12 ON 17 OCT 2005

FILE 'HCAPLUS' ENTERED AT 08:02:27 ON 17 OCT 2005

L47 188 S ?MGLI?

FILE 'REGISTRY' ENTERED AT 08:03:20 ON 17 OCT 2005

L48 STR  
L49 1 S L48  
L50 6880 S (MG AND LI)/ELS  
L51 381 S L50 NOT (AYS OR TIS OR PMS OR MNS OR MXS)/CI

FILE 'CASREACT' ENTERED AT 08:04:54 ON 17 OCT 2005

L52 0 S L51 AND L44

FILE 'REGISTRY' ENTERED AT 08:05:46 ON 17 OCT 2005

L53 258 S L51 NOT (N OR SI)/ELS  
L54 114 S L49 FUL  
SAV L54 SHIAO715A/A  
L55 27 S L54 AND L50  
L56 20 S L55 AND L53

FILE 'HCAPLUS' ENTERED AT 08:07:41 ON 17 OCT 2005

L57 33 S L56  
L58 206 S L47,L57

FILE 'REGISTRY' ENTERED AT 08:08:02 ON 17 OCT 2005

FILE 'HCAPLUS' ENTERED AT 08:08:02 ON 17 OCT 2005

SET SMARTSELECT ON  
L59 SEL L58 1- RN : 1756 TERMS  
SET SMARTSELECT OFF

FILE 'REGISTRY' ENTERED AT 08:08:09 ON 17 OCT 2005

L60 1756 S L59  
L61 0 S L26 SAM SUB=L60  
L62 STR L26  
L63 0 S L62 SAM SUB=L60  
L64 8467 S L50,L54-L56,L60  
L65 0 S L62 SAM SUB=L64  
L66 7 S L62 FUL SUB=L64  
SAV L66 SHIAL715B/A

FILE 'HCAPLUS' ENTERED AT 08:10:53 ON 17 OCT 2005

L67 6033 S L66  
L68 2 S L47 AND L67  
L69 1 S L68 NOT ROMGLIZONE  
L70 1 S L56 AND L67  
L71 1 S L69,L70 AND L1-L11  
L72 2 S L69,L70,L71

=> fil reg

FILE 'REGISTRY' ENTERED AT 08:13:07 ON 17 OCT 2005

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STRUCTURE FILE UPDATES: 16 OCT 2005 HIGHEST RN 865349-47-9

DICTIONARY FILE UPDATES: 16 OCT 2005 HIGHEST RN 865349-47-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

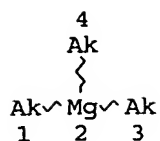
Structure search iteration limits have been increased. See HELP SLIMITS  
for details.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> d sta que l54

L48 STR



NODE ATTRIBUTES:  
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 DEFAULT ECLEVEL IS LIMITED

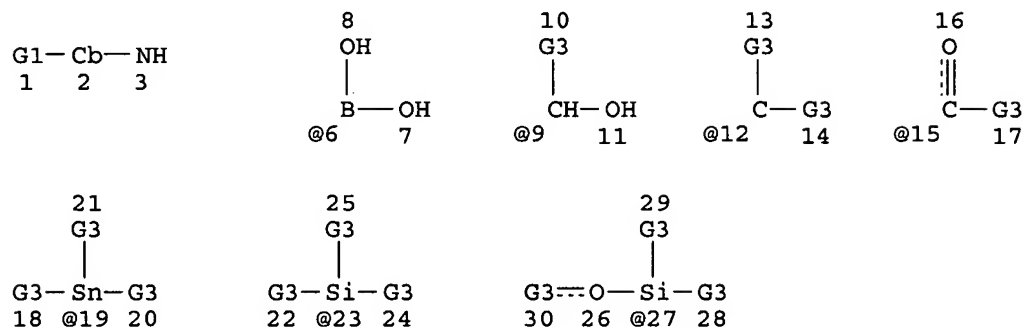
GRAPH ATTRIBUTES:  
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STEREO ATTRIBUTES: NONE  
 L54 114 SEA FILE=REGISTRY SSS FUL L48

100.0% PROCESSED 137963 ITERATIONS  
 SEARCH TIME: 00.00.01

114 ANSWERS

=> d 162  
 L62 HAS NO ANSWERS  
 L62 STR



VAR G1=6/9/12/AK/CY/15/19/23/27/X

VAR G3=AK/CY

NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED  
 ECOUNT IS M6-X10 C AT 2

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 28

STEREO ATTRIBUTES: NONE

=> fil hcaplus  
 FILE 'HCAPLUS' ENTERED AT 08:13:26 ON 17 OCT 2005  
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FILE COVERS 1907 - 17 Oct 2005 VOL 143 ISS 17  
FILE LAST UPDATED: 16 Oct 2005 (20051016/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all hitstr tot 172

L72 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN  
AN 2004:626042 HCAPLUS  
DN 141:260321  
ED Entered STN: 05 Aug 2004  
TI Halogen-magnesium exchange of m- and p-iodo or bromo-arenes bearing ortho-directing groups through ate complexes  
AU Xu, Jiayi; Jain, Nareshkumar; Sui, Zhihua  
CS Drug Discovery, Johnson & Johnson Pharmaceutical Research and Development, L.L.C., Raritan, NJ, 08869, USA  
SO Tetrahedron Letters (2004), 45(34), 6399-6402  
CODEN: TELEAY; ISSN: 0040-4039  
PB Elsevier  
DT Journal  
LA English  
CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
OS CASREACT 141:260321  
AB M- or p-Iodinated, or brominated phenoxy alcs. and phenols as well as halogenated indoles were subjected to halogen-magnesium exchange reactions with iso-Pr magnesium bromide or iso-Pr magnesium di-Bu lithium (i-PrMgnBu2Li) ate complexes. I-PrMgnBu2Li was superior to prevent ortho-metalation of these substituted arenes.  
ST iodoarene aldehyde magnesium halogen exchange alkylation; hydroxymethylarene prepn  
IT Exchange reaction  
(halogen-magnesium; preparation of disubstituted benzenes or ( $\alpha$ -hydroxybenzyl)indole via halogen-magnesium exchange of iodoarenes with magnesium-reagents followed by alkylation with aldehydes or allyl bromide)  
IT Alkylation  
(preparation of disubstituted benzenes or ( $\alpha$ -hydroxybenzyl)indole via halogen-magnesium exchange of iodoarenes with magnesium-reagents followed by alkylation with aldehydes or allyl bromide)  
IT Aldehydes, reactions  
Aryl halides  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of disubstituted benzenes or ( $\alpha$ -hydroxybenzyl)indole via halogen-magnesium exchange of iodoarenes with magnesium-reagents followed by alkylation with aldehydes or allyl bromide)

IT 100-52-7, Benzaldehyde, reactions 103-88-8 106-41-2,  
4-Bromophenol 106-95-6, Allylbromide, reactions 540-38-5, 4-Iodophenol  
591-20-8, 3-Bromophenol 622-50-4, 4-Iodoacetanilide 626-02-8,  
3-Iodophenol 630-19-3, 2,2-Dimethylpropanal 10075-50-0, 5-Bromoindole  
16066-91-4, 5-Iodoindole 29639-77-8 34743-88-9 67856-27-3  
67900-64-5 79906-55-1 115666-47-2, 6-Iodoindole 145073-42-3  
756488-21-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of disubstituted benzenes or ( $\alpha$ -hydroxybenzyl)indole via  
halogen-magnesium exchange of iodoarenes with magnesium-reagents  
followed by alkylation with aldehydes or allyl bromide)

IT 920-39-8, Isopropylmagnesium bromide 1068-55-9, Isopropylmagnesium  
chloride 15228-08-7 34376-14-2, (Diisopropylamino)isopropylmagnesium  
296802-58-9

RL: RGT (Reagent); RACT (Reactant or reagent)

(preparation of disubstituted benzenes or ( $\alpha$ -hydroxybenzyl)indole via  
halogen-magnesium exchange of iodoarenes with magnesium-reagents  
followed by alkylation with aldehydes or allyl bromide)

IT 102877-87-2P 108714-83-6P 146256-24-8P 146256-25-9P  
163258-61-5P 756488-22-9P 756488-23-0P 756488-24-1P 756488-25-2P  
756488-26-3P 756488-27-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of disubstituted benzenes or ( $\alpha$ -hydroxybenzyl)indole via  
halogen-magnesium exchange of iodoarenes with magnesium-reagents  
followed by alkylation with aldehydes or allyl bromide)

RE.CNT 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD  
RE

- (1) Abarbri, M; J Org Chem 2000, V65, P4618 HCAPLUS
- (2) Abarbri, M; Synlett 1999, P1577 HCAPLUS
- (3) Abarbri, M; Tetrahedron Lett 1999, V40, P7449 HCAPLUS
- (4) Anon; Grignard Reagents: New Developments 1999
- (5) Anon; Handbook of Grignard-Reagents 1996
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- (10) Boudier, A; Angew Chem, Int Ed 2000, V39, P4414
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- (15) Fukuhara, K; Am Chem Soc 2003, V125(23), P6884 HCAPLUS
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- (32) Rottlander, M; J Org Chem 1999, V64(4), P1080
- (33) Salteris, C; J Org Chem 1999, V64, P5589 HCAPLUS

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 (35) Salteris, C; Main Group Met Chem 1999, V22, P427 HCAPLUS  
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 (43) Yasuda, M; Synlett 1998, P899  
 (44) Yus, M; Chem Soc Rev 1996, P155 HCAPLUS

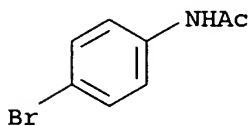
IT 103-88-8 622-50-4, 4-Iodoacetanilide

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of disubstituted benzenes or ( $\alpha$ -hydroxybenzyl)indole via halogen-magnesium exchange of iodoarenes with magnesium-reagents followed by alkylation with aldehydes or allyl bromide)

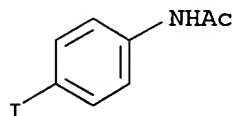
RN 103-88-8 HCAPLUS

CN Acetamide, N-(4-bromophenyl)- (9CI) (CA INDEX NAME)



RN 622-50-4 HCAPLUS

CN Acetamide, N-(4-iodophenyl)- (9CI) (CA INDEX NAME)



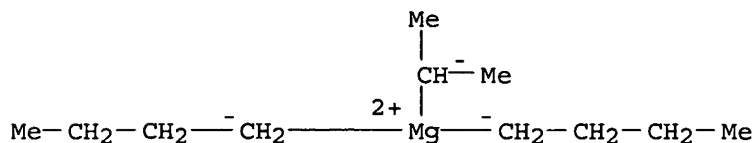
IT 296802-58-9

RL: RGT (Reagent); RACT (Reactant or reagent)

(preparation of disubstituted benzenes or ( $\alpha$ -hydroxybenzyl)indole via halogen-magnesium exchange of iodoarenes with magnesium-reagents followed by alkylation with aldehydes or allyl bromide)

RN 296802-58-9 HCAPLUS

CN Magnesate(1-), dibutyl(1-methylethyl)-, lithium (9CI) (CA INDEX NAME)



● Li<sup>+</sup>

IT 108714-83-6P

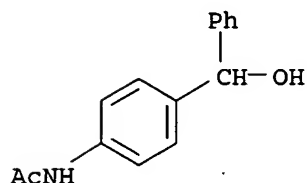
RL: SPN (Synthetic preparation); PREP (Preparation)



(preparation of disubstituted benzenes or ( $\alpha$ -hydroxybenzyl)indole via halogen-magnesium exchange of iodoarenes with magnesium-reagents followed by alkylation with aldehydes or allyl bromide)

RN 108714-83-6 HCAPLUS

CN Acetamide, N- [4-(hydroxyphenylmethyl)phenyl]- (9CI) (CA INDEX NAME)



L72 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:451671 HCAPLUS

DN 141:23307

ED Entered STN: 04 Jun 2004

TI Preparation of aryl intermediates such as arylboronic acids

IN Song, Jinhua J.; Tan, Zhulin; Yee, Nathan K.

PA Boehringer Ingelheim Pharmaceuticals, Inc., USA

SO U.S. Pat. Appl. Publ., 5 pp.

CODEN: USXXCO

DT Patent

LA English

IC ICM C07D207-46

INCL 548577000; 564395000; 260665000G

CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

FAN.CNT 1

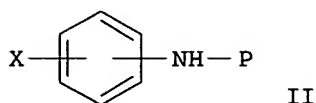
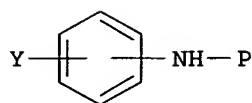
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004106807	A1	20040603	US 2003-715029	20031117 <--
	CA 2506913	AA	20040610	CA 2003-2506913	20031117 <--
	WO 2004048389	A1	20040610	WO 2003-US36685	20031117 <--
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	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW:				
	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	EP 1565477	A1	20050824	EP 2003-783591	20031117 <--
	R:				
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PRAI	US 2002-428618P	P	20021122		<--
	WO 2003-US36685	W	20031117		<--

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 2004106807	ICM	C07D207-46
	INCL	548577000; 564395000; 260665000G
US 2004106807	NCL	548/577.000
	ECLA	C07F005/02C
CA 2506913	ECLA	C07F005/02C

WO 2004048389 ECLA C07F005/02C  
 EP 1565477 ECLA C07F005/02C  
 OS CASREACT 141:23307  
 GI

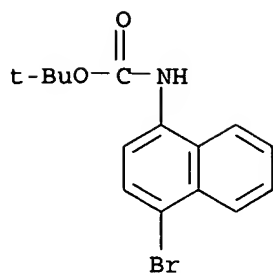
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- AB Disclosed are methods of making aryl intermediate compds. I [P = N-protecting group chemical suitable for Grignard reagents; Y = B(OH)<sub>2</sub>, CHR<sub>1</sub>OH, C(R<sub>1</sub>)<sub>2</sub>OH, etc.; R<sub>1</sub> = alkyl, aryl; Ph ring is optionally benzofused to form naphthyl] which are useful in the production of heteroaryl ureas. The compds. I are prepared in a one pot reaction comprising (1) reacting II [X = Br, I; the remaining substituents defined as above] with 2 equiv of R<sub>3</sub>MgLi (wherein R = alkyl) in a aprotic solvent at a temperature between -40° to 40°C; and (2) adding an electrophile such as B(Oalkyl)<sub>3</sub>, R<sub>1</sub>CHO; (R<sub>1</sub>)<sub>2</sub>CO, etc. to produce the compound I. Thus, treating BuMgCl with BuLi in THF followed by addition of N-Boc-4-bromo-1-aminonaphthalene, and subsequently adding B(OMe)<sub>2</sub><sub>3</sub> afforded 65% N-Boc-4-amino-1-naphthaleneboronic acid.
- ST arylboronic acid aryl intermediate prepn heteroaryl urea; naphthylboronic acid prepn intermediate heteroaryl urea
- IT Acids, preparation  
 Group IIIA element compounds  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (boronic acids; preparation of N-Boc-4-amino-1-naphthaleneboronic acid from N-Boc-1-amino-4-bromonaphthalene)
- IT 121-43-7, Trimethylborate **698370-68-2**  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of N-Boc-4-amino-1-naphthaleneboronic acid from N-Boc-1-amino-4-bromonaphthalene)
- IT **698370-58-0P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of N-Boc-4-amino-1-naphthaleneboronic acid from N-Boc-1-amino-4-bromonaphthalene)
- IT 109-99-9, Thf, uses  
 RL: NUU (Other use, unclassified); USES (Uses)  
 (solvent; preparation of N-Boc-4-amino-1-naphthaleneboronic acid from N-Boc-1-amino-4-bromonaphthalene)
- IT **698370-68-2**  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of N-Boc-4-amino-1-naphthaleneboronic acid from N-Boc-1-amino-4-bromonaphthalene)
- RN 698370-68-2 HCAPLUS
- CN Formic acid, 1,1-dimethylethyl ester, compd. with 1,1-dimethylethyl (4-bromo-1-naphthalenyl) carbamate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 168169-11-7  
 CMF C15 H16 Br N O2



CM 2

CRN 762-75-4

CMF C5 H10 O2

t-Bu-O-CHO

IT 698370-58-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of N-Boc-4-amino-1-naphthaleneboronic acid from  
 N-Boc-1-amino-4-bromonaphthalene)

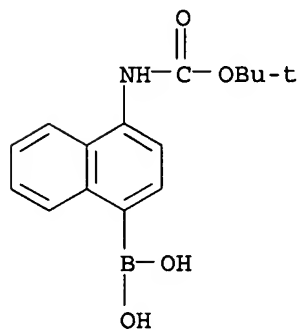
RN 698370-58-0 HCAPLUS

CN Formic acid, 1,1-dimethylethyl ester, compd. with C-(1,1-dimethylethyl)  
 (4-borono-1-naphthalenyl)carbamate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 294852-07-6

CMF C15 H18 B N O4



CM 2

CRN 762-75-4

CMF C5 H10 O2

t-Bu-O-CHO

=> => fil casreact.

FILE 'CASREACT' ENTERED AT 08:17:08 ON 17 OCT 2005  
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT  
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FILE CONTENT:1840 - 16 Oct 2005 VOL 143 ISS 16

New CAS Information Use Policies, enter HELP USAGETERMS for details.

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*****
*
*      CASREACT now has more than 9.2 million reactions      *
*
*****
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Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d sta que

L45 13 SEA FILE=CASREACT ABB=ON PLU=ON ?MGLI?  
L48 STR

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  4
  Ak
  }
Ak^Mg^Ak
1  2  3
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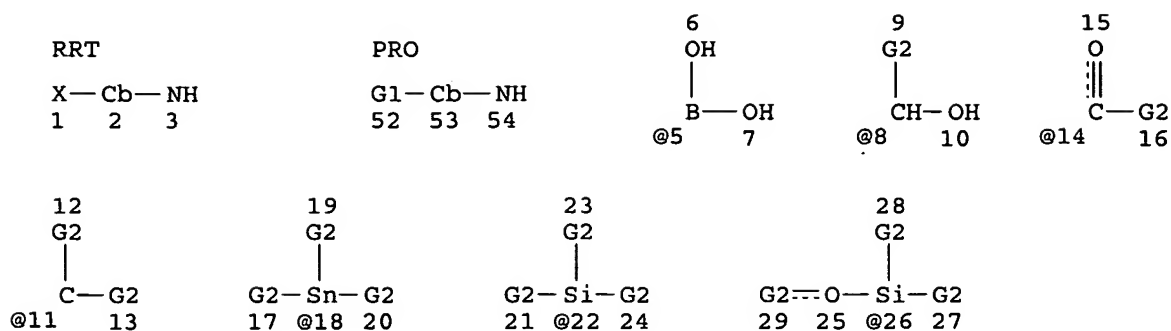
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DEFAULT ECLEVEL IS LIMITED

#### GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 4

#### STEREO ATTRIBUTES: NONE

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L51 381 SEA FILE=REGISTRY ABB=ON PLU=ON L50 NOT (AYS OR TIS OR PMS
      OR MNS OR MXS)/CI
L53 258 SEA FILE=REGISTRY ABB=ON PLU=ON L51 NOT (N OR SI)/ELS
L54 114 SEA FILE=REGISTRY SSS FUL L48
L55 27 SEA FILE=REGISTRY ABB=ON PLU=ON L54 AND L50
L56 20 SEA FILE=REGISTRY ABB=ON PLU=ON L55 AND L53
L74 8 SEA FILE=CASREACT ABB=ON PLU=ON L56
L75 17 SEA FILE=CASREACT ABB=ON PLU=ON (L45 OR L74)
L77 STR
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VAR G1=5/8/11/AK/CY/14/18/22/26

VAR G2=AK/CY

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS M6-X10 C AT 2

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 31

STEREO ATTRIBUTES: NONE

L79 2 SEA FILE=CASREACT SUB=L75 SSS FUL L77 ( 2 REACTIONS)

100.0% DONE 484 VERIFIED 2 HIT RXNS 2 DOCS

SEARCH TIME: 00.00.01

=> d bib abs fhlt retable tot

L79 ANSWER 1 OF 2 CASREACT COPYRIGHT 2005 ACS on STN

AN 141:260321 CASREACT

TI Halogen-magnesium exchange of m- and p-iodo or bromo-arenes bearing ortho-directing groups through ate complexes

AU Xu, Jiayi; Jain, Nareshkumar; Sui, Zhihua

CS Drug Discovery, Johnson & Johnson Pharmaceutical Research and Development, L.L.C., Raritan, NJ, 08869, USA

SO Tetrahedron Letters (2004), 45(34), 6399-6402

CODEN: TELEAY; ISSN: 0040-4039

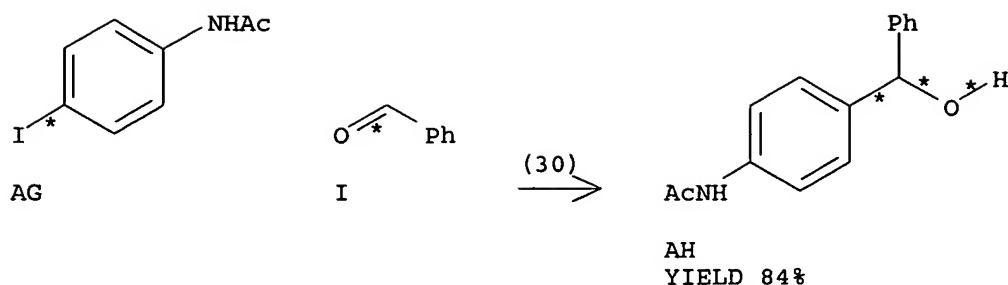
PB Elsevier

DT Journal

LA English

AB M- or p-Iodinated, or brominated phenoxy alcs. and phenols as well as halogenated indoles were subjected to halogen-magnesium exchange reactions with iso-Pr magnesium bromide or iso-Pr magnesium di-Bu lithium (i-PrMgBu<sub>2</sub>Li) ate complexes. I-PrMgBu<sub>2</sub>Li was superior to prevent ortho-metalation of these substituted arenes.

RX(30) OF 37 AG + I ==> AH



RX(30) RCT AG 622-50-4

STAGE(1)

RGT N 296802-58-9 Magnesate(1-), dibutyl(1-methylethyl)-, lithium  
 SOL 109-99-9 THF  
 CON SUBSTAGE(1) 30 minutes, -10 deg C  
 SUBSTAGE(2) -10 deg C -> -78 deg C

STAGE(2)

RCT I 100-52-7  
 SOL 109-99-9 THF  
 CON 1 hour, -10 deg C

STAGE(3)

RGT E 12125-02-9 NH4Cl  
 SOL 7732-18-5 Water

PRO AH 108714-83-6

NTE other reagent gave lower yield

RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
=====	=====	=====	=====	=====	=====
Abarbri, M	2000	65	4618	J Org Chem	CAPLUS
Abarbri, M	1999		1577	Synlett	CAPLUS
Abarbri, M	1999	40	7449	Tetrahedron Lett	CAPLUS
Anon	1999			Grignard Reagents: N	
Anon	1996			Handbook of Grignard	
Ashby, E	1974	39	3258	J Org Chem	CAPLUS
Avolio, S	1999		1820	Synlett	CAPLUS
Berillon, L	1998		1359	Synlett	CAPLUS
Boudier, A	2000	112	4584	Angew Chem	
Boudier, A	2000	39	4414	Angew Chem, Int Ed	
Boymond, L	1998	110	1801	Angew Chem	
Boymond, L	1998	37	1701	Angew Chem, Int Ed	CAPLUS
Castaldi, G	1992			EP 491326	CAPLUS
Dehmel, F	2000		345	Synlett	CAPLUS
Fukuhara, K	2003	125	6884	Am Chem Soc	CAPLUS
Harada, T	1993	58	4897	J Org Chem	CAPLUS
Ide, M	1999	72	2491	Bull Chem Soc Jpn	CAPLUS
Ide, M	1998		936	Synlett	CAPLUS
Iida, T				JP 2000024613	CAPLUS
Inoue, A	2001	66	4333	J Org Chem	CAPLUS
Kamienski, C	1974			US 3847883	CAPLUS
Kitagawa, K	2000	112	2594	Angew Chem	

Kitagawa, K	2000	39	2481	Angew Chem, Int Ed	CAPLUS
Klump, G	1986	105	1	Recl Trav Chim Pays-	CAPLUS
Kondo, Y	1996	108	818	Angew Chem	
Kondo, Y	1996	35	736	Angew Chem, Int Ed E	CAPLUS
Kondo, Y	1994	59	4717	J Org Chem	CAPLUS
Nicolaou, K	1998	37	2717	Angew Chem, Int Ed	CAPLUS
Richey, H	1990	9	1778	Organometallics	CAPLUS
Richey, H	1985	26	275	Tetrahedron Lett	CAPLUS
Rottlander, M	2000	6	767	Chem Eur J	CAPLUS
Rottlander, M	1999	64	1080	J Org Chem	
Salteris, C	1999	64	5589	J Org Chem	CAPLUS
Salteris, C	1999	590	63	J Organomet Chem	CAPLUS
Salteris, C	1999	22	427	Main Group Met Chem	CAPLUS
Snieckus, V	1990	90	879	Chem Rev	CAPLUS
Thibonnet, J	2000	41	3319	Tetrahedron Lett	CAPLUS
Uchiyama, M	1996	118	8733	J Am Chem Soc	CAPLUS
Uchiyama, M	1998	120	4934	J Am Chem Soc	CAPLUS
Varchi, G	2000	56	2727	Tetrahedron	CAPLUS
Wakefield, B	1995			Organomagnesium Meth	
Yasuda, M	1998	71	1417	Bull Chem Soc Jpn	CAPLUS
Yasuda, M	1998		899	Synlett	
Yus, M	1996		155	Chem Soc Rev	CAPLUS

L79 ANSWER 2 OF 2 CASREACT COPYRIGHT 2005 ACS on STN

AN 141:23307 CASREACT

TI Preparation of aryl intermediates such as arylboronic acids

IN Song, Jinhua J.; Tan, Zhulin; Yee, Nathan K.

PA Boehringer Ingelheim Pharmaceuticals, Inc., USA

SO U.S. Pat. Appl. Publ., 5 pp.

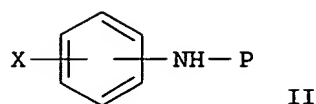
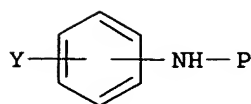
CODEN: USXXCO

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004106807	A1	20040603	US 2003- <del>715029</del>	20031117
	CA 2506913	AA	20040610	CA 2003-2506913	20031117
	WO 2004048389	A1	20040610	WO 2003-US36685	20031117
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	EP 1565477	A1	20050824	EP 2003-783591	20031117
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
PRAI	US 2002-428618P		20021122		
	WO 2003-US36685		20031117		
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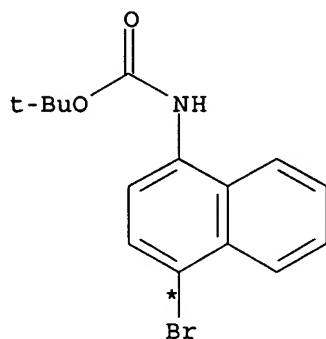


AB Disclosed are methods of making aryl intermediate compds. I [P = N-protecting group chemical suitable for Grignard reagents; Y = B(OH)<sub>2</sub>, CHR<sub>1</sub>OH, C(R<sub>1</sub>)<sub>2</sub>OH, etc.; R<sub>1</sub> = alkyl, aryl; Ph ring is optionally benzofused to form naphthyl] which are useful in the production of heteroaryl ureas. The compds. I are prepared in a one pot reaction comprising (1) reacting II [X = Br, I; the remaining substituents defined as above] with 2 equiv of R<sub>3</sub>MgLi (wherein R = alkyl) in a aprotic solvent at a temperature between -40° to 40°C; and (2) adding an electrophile such as B(Oalkyl)<sub>3</sub>, R<sub>1</sub>CHO; (R<sub>1</sub>)<sub>2</sub>CO, etc. to produce the compound I. Thus, treating BuMgCl with BuLi in THF followed by addition of N-Boc-4-bromo-1-aminonaphtalene, and subsequently adding B(OMe)<sub>2</sub> afforded 65% N-Boc-4-amino-1-naphthaleneboronic acid.

RX(1) OF 1      A ==> B

t-Bu-O-CHO

A: CM 1



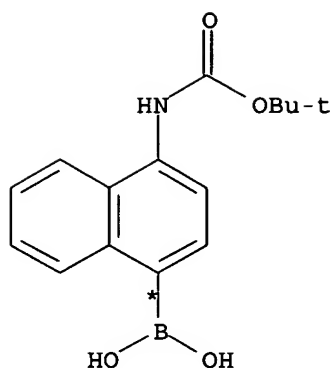
A: CM 2



t-Bu-O-CHO

B: CM 1  
YIELD 65%





B: CM 2  
YIELD 65%

RX(1)

STAGE(1)

RGT C 109-72-8 BuLi, D 693-04-9 BuMgCl  
SOL 109-99-9 THF, 110-54-3 Hexane  
CON SUBSTAGE(1) room temperature -> -5 deg C  
SUBSTAGE(2) <0 deg C  
SUBSTAGE(3) 0.5 hours, 0 deg C  
SUBSTAGE(4) 0 deg C -> -5 deg C

STAGE(2)

RCT A 698370-68-2  
SOL 109-99-9 THF  
CON SUBSTAGE(1) <0 deg C  
SUBSTAGE(2) 0.5 hours, 0 deg C

STAGE(3)

RGT E 67-56-1 MeOH

STAGE(4)

RGT F 121-43-7 Me borate  
CON SUBSTAGE(1) -5 deg C  
SUBSTAGE(3) 2 hours, 0 deg C

STAGE(5)

RGT G 12125-02-9 NH4Cl  
SOL 7732-18-5 Water

PRO B 698370-58-0

=> d his

(FILE 'HOME' ENTERED AT 07:16:36 ON 17 OCT 2005)  
SET COST OFF

FILE 'HCAPLUS' ENTERED AT 07:16:46 ON 17 OCT 2005

L1 1 S US20040106807/PN OR (US2003-715029# OR WO2003-US36685 OR US20  
E SONG/AU  
L2 2 S E3

jan delaval - 17 october 2005

L3           E SONG J/AU  
 370 S E3,E13,E14  
 L4           229 S E11  
             E SONG JIN/AU  
 L5           23 S E3,E29  
             E SONG JINHUA/AU  
 L6           27 S E3,E4  
             E TAN/AU  
 L7           1 S E3  
             E TAN Z/AU  
 L8           69 S E3,E13  
             E TAN SHU/AU  
             E TAN ZHU/AU  
 L9           1 S E3  
 L10          11 S E14  
             E YEE/AU  
             E YEE N/AU  
 L11          61 S E3-E5,E8-E11  
             SEL RN L1

FILE 'REGISTRY' ENTERED AT 07:19:35 ON 17 OCT 2005

L12           4 S E1-E4

FILE 'HCAPLUS' ENTERED AT 07:20:23 ON 17 OCT 2005

L13          768 S L2-L11 NOT L1  
 L14          35 S L13 AND (BOEHRIN? OR BOHRIN?)/PA,CS  
 L15          3 S L13 AND BENZEN?/SC,SX  
 L16          1 S L13 AND GRIGNARD  
             E GRIGNARD/CT  
 L17          19700 S E8+OLD,NT OR E13+OLD,NT OR E20+OLD,NT OR E22+OLD,NT  
 L18          9760 S E3-E29  
             E E8+ALL  
             E E8+ALL  
 L19          4 S L13 AND L17,L18  
 L20          36 S L14-L16,L19  
             SEL RN

FILE 'REGISTRY' ENTERED AT 07:25:06 ON 17 OCT 2005

L21          606 S E1-E606  
 L22          8 S L21 AND MG/ELS  
 L23          8 S L21 AND LI/ELS  
 L24          126 S L21 AND C6-C6/ES  
 L25          71 S L24 AND C6/ES  
 L26          STR  
 L27          0 S L26 CSS  
 L28          STR L26  
 L29          0 S L28 CSS  
 L30          STR L28  
 L31          1 S L30 CSS

FILE 'CASREACT' ENTERED AT 07:44:50 ON 17 OCT 2005

L32          STR  
 L33          0 S L32 CSS  
 L34          SCR 1120  
 L35          0 S L32 AND L34 CSS SAM  
 L36          SCR 1918  
 L37          1 S L32 AND L34 AND L36 CSS SAM  
 L38          SCR 1989 OR 1990  
 L39          0 S L32 AND L34 AND L38 CSS SAM  
 L40          SCR 1989 AND 1990

L41 0 S L32 AND L34 AND L40 CSS SAM  
 L42 0 S L32 AND L34 AND L40 SAM  
 L43 1 S L32 AND L34 AND L38 SAM  
 L44 1 S L1  
 L45 13 S ?MGLI?  
 L46 0 S L32 SAM SUB=L45

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FILE 'REGISTRY' ENTERED AT 07:57:59 ON 17 OCT 2005

FILE 'CASREACT' ENTERED AT 07:58:10 ON 17 OCT 2005  
 SET SMARTSELECT ON  
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FILE 'REGISTRY' ENTERED AT 07:58:12 ON 17 OCT 2005

L47 FILE 'HCAPLUS' ENTERED AT 08:02:27 ON 17 OCT 2005  
 188 S ?MGLI?

L48 FILE 'REGISTRY' ENTERED AT 08:03:20 ON 17 OCT 2005  
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 L49 1 S L48  
 L50 6880 S (MG AND LI)/ELS  
 L51 381 S L50 NOT (AYS OR TIS OR PMS OR MNS OR MXS)/CI

L52 FILE 'CASREACT' ENTERED AT 08:04:54 ON 17 OCT 2005  
 0 S L51 AND L44

L53 FILE 'REGISTRY' ENTERED AT 08:05:46 ON 17 OCT 2005  
 258 S L51 NOT (N OR SI)/ELS  
 L54 114 S L49 FUL  
 SAV L54 SHIAO715A/A  
 L55 27 S L54 AND L50  
 L56 20 S L55 AND L53

L57 FILE 'HCAPLUS' ENTERED AT 08:07:41 ON 17 OCT 2005  
 33 S L56  
 L58 206 S L47,L57

FILE 'REGISTRY' ENTERED AT 08:08:02 ON 17 OCT 2005

L59 FILE 'HCAPLUS' ENTERED AT 08:08:02 ON 17 OCT 2005  
 SET SMARTSELECT ON  
 SEL L58 1- RN : 1756 TERMS  
 SET SMARTSELECT OFF

L60 FILE 'REGISTRY' ENTERED AT 08:08:09 ON 17 OCT 2005  
 1756 S L59  
 L61 0 S L26 SAM SUB=L60  
 L62 STR L26  
 L63 0 S L62 SAM SUB=L60  
 L64 8467 S L50,L54-L56,L60  
 L65 0 S L62 SAM SUB=L64  
 L66 7 S L62 FUL SUB=L64  
 SAV L66 SHIAL715B/A

FILE 'HCAPLUS' ENTERED AT 08:10:53 ON 17 OCT 2005

L67 6033 S L66  
L68 2 S L47 AND L67  
L69 1 S L68 NOT ROMGLIZONE  
L70 1 S L56 AND L67  
L71 1 S L69,L70 AND L1-L11  
L72 2 S L69,L70,L71

FILE 'REGISTRY' ENTERED AT 08:13:07 ON 17 OCT 2005

FILE 'HCAPLUS' ENTERED AT 08:13:26 ON 17 OCT 2005

FILE 'CASREACT' ENTERED AT 08:14:04 ON 17 OCT 2005

L73 14 S L54  
L74 8 S L56  
L75 17 S L45,L74  
L76 0 S L32 SAM SUB=L75  
L77 STR L32  
L78 0 S L77 SAM SUB=L75  
L79 2 S L77 FUL SUB=L75  
SAV L79 SHIAO715C/A

FILE 'CASREACT' ENTERED AT 08:17:08 ON 17 OCT 2005

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